JS 1/19/22
RJA 2/16/22

Ecotox Report for Case # P-18-0020

General

[redacted]

Report Status: Complete
Status Date: 01/28/2019
CRSS Date: 10/23/2017
SAT Date: 10/24/2017
SAT Chair: Legacy Placeholder
Consolidated PMN: N
Consolidated Set:
Ecotox Related Cases:
Health Related Cases: ANALOGS; [redacted]
Submitter: Myriant Corporation
CAS Number: None
Chemical Name: Butanedioic acid, polymer with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol, 2,5-furandione and 1,3-propanediol, 3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-inden-5(or 6)-yl ester
Use: [redacted] and [redacted]. Analog [redacted] (by terminal groups).
Trade Name: Myribond(R) DX
PV-max(kg/yr): 500000.0000
Ecotox Assessor: Gallagher, Jeffrey

Fate Summary Statement

Fate Summary Statement: P-18-0020

FATE: Estimations for typical MW polymer, MW = 539, C31H38O8

Liquid with MP < 25 °C (E)
log Kow = 6.72 (E)
S = 0.019
mg/L at 25 °C (E)
VP < 1.0E-6 torr at 25 °C (E)
BP > 400 °C
(E)

H < 1.00E-8 (E)
log Koc = 7.89 (E)
log Fish BCF = 4.10
(13,000) (E)
log Fish BAF = 1.15 (14) (E)
POTW removal (%) = 90
via sorption
Time for complete ultimate aerobic biodeg > mo

Sorption to soils/sediments = v.strong
PBT Potential: P3B1

*CEB FATE: Migration to ground water = negl
Bioconcentration
factor to be put into E-FAST: 14

PMN Material:
Overall
wastewater treatment removal is 90% via sorption.
Sorption to sludge
is strong based on the STP model output.
Air Stripping
(Volatilization to air) is negligible based on the estimated
physical-chemical properties.
Removal by biodegradation in
wastewater treatment is negligible to moderate, with uncertainty. There was uncertainty due to the fact that the PMN is a polymer with a variable chemical structure. Depending on the structure and the terminated ends, the smaller pieces may biodegrade in wastewater treatment plants.

The aerobic aquatic biodegradation half-life is greater than months
based on structure.
The anaerobic aquatic biodegradation half-life
is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.

Sorption to soil and sediment is very strong based on the
estimated physical-chemical properties.
Migration to groundwater is
negligible based on the estimated physical-chemical properties.
PMN
Material:
High Persistence (P3) is based on the estimated anaerobic
biodegradation half-life.
Low Bioaccumulation potential (B1) is

based on the estimated Bioaccumulation factor (BAF).

Bioconcentration/Bioaccumulation factor to be put into E-Fast:
14

Physical Chemical Information

Molecular Weight:	535.00		
Wt% < 500:	35.00	**Wt% < 1000:**	57.00
Physical State - Neat:	Liquid		
Melting Point:		**Melting Point (est):**	
MP (EPI):	20.00		
Vapor Pressure:		**Vapor Pressure (est):**	<0.000001
VP (EPI):	9.55e-010		
Water Solubility:		**Water Solubility (est):**	0.000019
Water Solubility (EPI):			
Henry's Law::	1.00e-008		
Log Koc:		**Log Koc (EPI):**	7.89
Log Kow:		**Log Kow (EPI):**	6.72
Log Kow Comment:			

SAT Concern Level

Ecotox Rating (1):	1
Ecotox Rating Comment (1):	
Ecotox Rating (2):	
Ecotox Rating Comment (2):	
Ecotox Route of Exposure:	No releases to water

Ecotox Comments

Exposure Based Review (Eco):	N
Ecotox Comments:	
Exposure Based Testing:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
3	1	1	

Eco-Toxicity Comment:

Fate Ratings

Removal in WWT/POTW (Overall): 90

Condition	Rating Values	Rating Description 1	2	3	4	Comment
Fish BCF:	12500.0000					
Log Fish BCF:	4.10					
WWT/POTW Sorption:	3	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	4	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	4	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	4	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
			Hours	Days	>= Months	

Removal in WWT/POTW (Overall):	90					
Condition	**Rating Values**	**Rating Description** **1**	**2**	**3**	**4**	**Comment**
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes				
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	1	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	1	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio Comments: Fate
study summaries are available. Fish log BAF = 1.15 (14).

Fate Comments: PMN Material:
Overall
wastewater treatment removal is 90% via sorption.
Sorption to sludge
is strong based on the STP model output.
Air Stripping
(Volatilization to air) is negligible based on the estimated physical-chemical properties.
Removal by biodegradation in
wastewater treatment is negligible to moderate, with uncertainty. There was uncertainty due to the fact that the PMN is a polymer with a variable chemical structure. Depending on the structure and the terminated ends, the smaller pieces may biodegrade in wastewater treatment plants.

The aerobic aquatic biodegradation half-life is greater than months based on structure.
The anaerobic aquatic biodegradation half-life
is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or

Removal in WWT/POTW (Overall): Condition	90 Rating Values	Rating Description 1	2	3	4	Comment
		equal to the aerobic biodegradation half-life. Sorption to soil and sediment is very strong based on the estimated physical-chemical properties. Migration to groundwater is negligible based on the estimated physical-chemical properties. PMN Material: High Persistence (P3) is based on the estimated anaerobic biodegradation half-life. Low Bioaccumulation potential (B1) is based on the estimated Bioaccumulation factor (BAF). Bioconcentration/Bioaccumulation factor to be put into E-Fast: 14				

Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)
Daphnid	48-h	LC50	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)
Green Algae	96-h	EC50	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)
Fish	-	Chronic Value	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)
Daphnid	-	Chronic Value	*		

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)
Green Algae	-	Chronic Value	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)

Ecotox Value Comments: Predictions are based on QSARs for esters (ECOSAR V2.0; assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000); Log Kow = 6.72 (P, 538 MW); liquid with an unknown MP (P); S = 0.02 mg/L (P, 538 MW); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L.

Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):				Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.
Chronic Aquatic (ppb):				Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.

Factors	Values	Comments
SARs:	Esters	
SAR Class:	Esters-insoluble	
TSCA NCC Category?	Esters	

Recommended Testing:

Ecotox Factors Environmental

Comments: Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-releationships-ecosar-predictive-model); specifically the QSAR for esters (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000). Acute and chronic toxicity values estimated for fish, aquatic invertebrates, and algae are all no effects at saturation. These toxicity values indicate that the new chemical substance is expected to have a low environmental hazard. Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.

Environmental Risk: Risks to the environment from acute

and chronic exposure are not expected at any concentration of the new chemical substance soluble in the water (i.e., no effects at saturation).

Comments/Telephone Log

Artifact	Update/Upload Time
[redacted]	[redacted]